

On the stability regions of implicit linear multistep methods

Lajos Lóczi*

April 29, 2014

Abstract

If we apply the accepted definition to determine the stability region of implicit linear multistep or implicit multiderivative multistep methods, we find in many cases that there are some isolated points of stability within their region of instability. Isolated stability points can be present when the leading coefficient of the characteristic polynomial of the implicit method vanishes. These points cannot be detected by the well-known root locus method, and their existence renders many results about stability regions contradictory. We suggest that the definition of the stability region should exclude such singular points.

1 Introduction

The aim of this short note is to point out the presence of certain isolated points of stability within the region of instability of some common implicit numerical methods. We argue that these points should not be included in the definition of the stability region.

Stability properties of a broad class of numerical methods (including Runge–Kutta methods, linear multistep methods, or multistep multiderivative methods) for solving initial value problems of the form

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0 \quad (1)$$

can be analyzed by studying the stability region of the method. When an s -stage k -step method ($s \geq 1$, $k \geq 1$ fixed positive integers) with constant step-size $h > 0$ is applied to the

*lajos.loczi@kaust.edu.sa

King Abdullah University of Science and Technology (KAUST), Saudi Arabia

linear test equation $y' = \lambda y$ ($\lambda \in \mathbb{C}$ fixed, $y(0) = y_0$ given), the method yields a numerical solution $(y_n)_{n \in \mathbb{N}}$ that satisfies a recurrence relation of the form [1]

$$\begin{cases} \sum_{j=0}^s \sum_{\ell=0}^k a_{j,\ell} \mu^j y_{n+\ell} = 0, & n \in \mathbb{N}, \\ a_{j,\ell} \in \mathbb{R}, \quad \sum_{j=0}^s |a_{j,k}| > 0, \quad \mu := h\lambda. \end{cases} \quad (2)$$

The characteristic polynomial associated with the method takes the form

$$\Phi(\zeta, \mu) := \sum_{j=0}^s \sum_{\ell=0}^k a_{j,\ell} \mu^j \zeta^\ell \quad (\zeta \in \mathbb{C}, \mu \in \mathbb{C}). \quad (3)$$

The stability region of the method is defined [3] as

$$\begin{aligned} \mathcal{S} := \{ \mu \in \mathbb{C} : \text{all roots } \zeta_m(\mu) \text{ of } \zeta \mapsto \Phi(\zeta, \mu) \text{ satisfy } |\zeta_m(\mu)| \leq 1, \\ \text{and multiple roots satisfy } |\zeta_m(\mu)| < 1 \} \end{aligned} \quad (4)$$

(in [1], $\mu \in \overline{\mathbb{C}}$ is present in the definition instead of $\mu \in \mathbb{C}$). It is known [1, 3] that

$$\text{the numerical solution } y_n \text{ for all possible initial values } y_0, y_1, \dots, y_{k-1} \text{ and } h > 0 \text{ fixed} \quad (5)$$

remains bounded as $n \rightarrow +\infty$ if and only if $\mu \in \mathcal{S}$.

Example 1.1 A linear k -step method [2, 3] approximating the solution of the initial value problem (1) can be written as

$$\sum_{\ell=0}^k (\alpha_\ell y_{n+\ell} - h\beta_\ell f_{n+\ell}) = 0, \quad (6)$$

where the $\alpha_\ell \in \mathbb{R}$ and $\beta_\ell \in \mathbb{R}$ ($\ell = 0, \dots, k$) numbers are the suitably chosen coefficients of the method, $\alpha_k \neq 0$, t_m is defined as $t_0 + mh$ ($m \in \mathbb{N}$), and f_m stands for $f(t_m, y_m)$. The numerical solution y_n approximates the exact solution y at time t_n . For $k = 1$ we have a one-step method, while for $k \geq 2$ the scheme is called a multistep method. The method is implicit, if $\beta_k \neq 0$. By setting

$$\varrho(\zeta) := \sum_{\ell=0}^k \alpha_\ell \zeta^\ell \quad \text{and} \quad \sigma(\zeta) := \sum_{\ell=0}^k \beta_\ell \zeta^\ell,$$

the associated characteristic polynomial is $\Phi(\zeta, \mu) = \varrho(\zeta) - \mu\sigma(\zeta)$.

Example 1.2 *Multiderivative multistep methods (or generalized multistep methods) extend the above class of methods by evaluating the derivatives of f at certain points as well. For example, a second derivative k -step method [3] has the form*

$$\sum_{\ell=0}^k (\alpha_\ell y_{n+\ell} - h\beta_\ell f_{n+\ell} - h^2\gamma_\ell g_{n+\ell}) = 0,$$

where $g_m := g(t_m, y_m)$ with $g(t, y) := \partial_1 f(t, y) + f(t, y) \cdot \partial_2 f(t, y)$, and the method is determined by the α_ℓ ($\alpha_k \neq 0$), β_ℓ and γ_ℓ real coefficients. The associated characteristic polynomial is now $\Phi(\zeta, \mu) = \sum_{\ell=0}^k (\alpha_\ell - \mu\beta_\ell - \mu^2\gamma_\ell)\zeta^\ell$.

2 Vanishing leading coefficient of the characteristic polynomial

The characteristic polynomial of the implicit Euler method with $s = k = 1$ is $\Phi(\zeta, \mu) = \zeta - 1 - \mu\zeta$. Now $1 \in \mathcal{S}$ because (4) is satisfied vacuously. For $\mu \neq 1$, $\Phi(\zeta, \mu) = 0$ if and only if $\zeta = 1/(1 - \mu)$. Hence

$$\mathcal{S} = \{\mu \in \mathbb{C} : |\mu - 1| \geq 1\} \cup \mathcal{E} \quad (7)$$

with $\mathcal{E} = \{1\}$. In particular, $1 \in \partial\mathcal{S}$, the boundary of \mathcal{S} .

Motivated by the above example, let us rewrite Φ in (3) as $\Phi(\zeta, \mu) =: \sum_{\ell=0}^k C_\ell(\mu)\zeta^\ell$ with suitable polynomials C_ℓ . The leading coefficient C_k does not vanish identically because of the assumption $\sum_{j=0}^s |a_{j,k}| > 0$ in (2), or $\alpha_k \neq 0$ in Examples 1.1 and 1.2. For implicit methods, C_k is a polynomial of degree at least 1, so the finite set

$$\mathcal{E} := \{\mu \in \mathbb{C} : C_k(\mu) = 0\} \quad (8)$$

is non-empty. Besides the implicit Euler method, there are plenty of examples of classical implicit numerical methods when all the complex roots of the polynomial $\Phi(\cdot, \mu^*)$ have modulus strictly less than 1 for some $\mu^* \in \mathcal{E}$, hence $\mu^* \in \mathcal{S}$.

Example 2.1 *The characteristic polynomial of the 2-step BDF method [3] is $\Phi(\zeta, \mu) = 3\zeta^2 - 4\zeta + 1 - 2\zeta^2\mu$. Its stability region is depicted in Figure 1. Now $\mathcal{E} = \{3/2\} \subset \mathcal{S}$, because the unique root of $\Phi(\zeta, 3/2) = 0$ is $\zeta = 1/4$.*

Example 2.2 *One can easily check that, for example, for several other BDF methods [3], implicit Adams methods [3], or Enright methods [3] (see Figure 2) we have the inclusion $\mathcal{E} \subset \mathcal{S}$.*

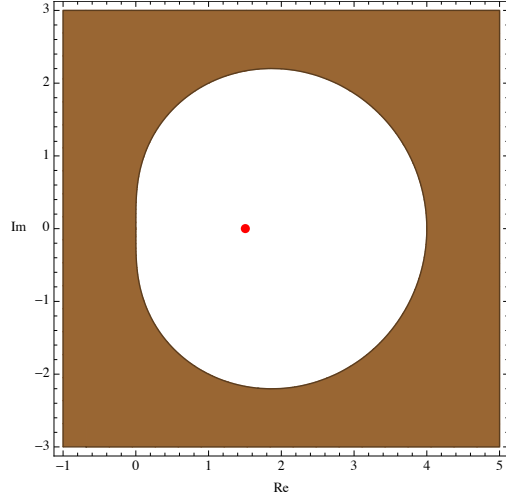


Figure 1: The stability region of the 2-step BDF method is shown in brown and red. The red dot is the unique element of $\mathcal{S} \cap \mathcal{E} = \{3/2\}$.

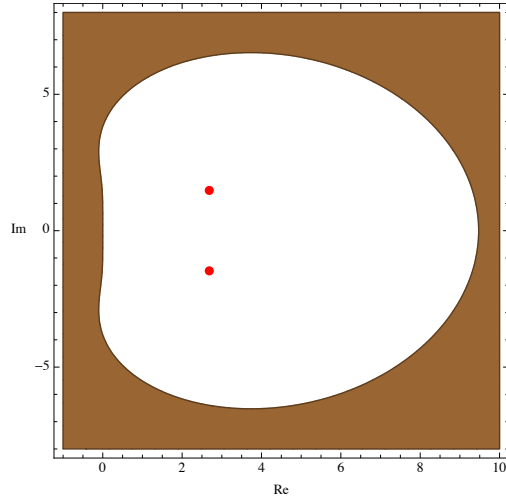


Figure 2: The stability region of the 3-step Enright method (member of the family presented in Example 1.2) is shown in brown and red. Now we have $\Phi(\zeta, \mu) = \left(\frac{19\mu^2}{180} - \frac{307\mu}{540} + 1\right)\zeta^3 + \left(-\frac{19\mu}{40} - 1\right)\zeta^2 + \frac{\mu}{20}\zeta - \frac{7\mu}{1080}$, and $\mathcal{E} = \{(307 \pm i\sqrt{28871})/114\}$. The two red dots represent the set $\mathcal{E} \subset \mathcal{S}$.

Now we show some consequences of the definition (4).

Observation 1. When the implicit Euler method is interpreted as a Runge–Kutta method, its stability function is defined as $R(z) := 1/(1-z)$ for $1 \neq z \in \mathbb{C}$. By definition, the stability region of a Runge–Kutta method is

$$\{z \in \mathbb{C} : |R(z)| \leq 1\} = \{z \in \mathbb{C} : |z - 1| \geq 1\},$$

which set is different from the stability region given in (7). We would have a similar discrepancy for example for the trapezoidal method when it is interpreted as a Runge–Kutta method or as a multistep method with $k = 1$.

Observation 2. Notice that elements of the set \mathcal{E} already pose a slight inconsistency in the equivalence (5), since the order of the recurrence relation corresponding to any $\mu \in \mathcal{E}$ is strictly less than k , hence y_{k-1} cannot be chosen appropriately. Moreover, recursions with vanishing leading terms can be quite unstable with respect to small perturbations of the coefficients, which renders the numerical method with this specific step-size $h > 0$ practically useless. As an example, let us consider the second order recursion corresponding to the 2-step BDF method $(3-2\mu)y_{n+2} - 4y_{n+1} + y_n = 0$. For $\mu = 3/2$, $\lim_{n \rightarrow +\infty} y_n = 0$ for any starting value y_0 , but for small $\varepsilon > 0$ and $0 < |\mu - 3/2| < \varepsilon$, the sequence $|y_n|$ quickly “blows up” for generic starting values, since the absolute value of one root of the characteristic polynomial $(3 - 2\mu)\zeta^2 - 4\zeta + 1 = 0$ is huge.

Observation 3. One way to study \mathcal{S} in the complex plane is to depict the root locus curve corresponding to the method. For methods in Example 1.1, Φ is linear in μ , so $\Phi(\zeta, \mu) = 0$ implies $\mu = \varrho(\zeta)/\sigma(\zeta)$ (for $\sigma(\zeta) \neq 0$). The root locus curve is then the parametric curve $[0, 2\pi) \ni \vartheta \mapsto \mu(\vartheta)$ with

$$\mu(\vartheta) := \frac{\varrho(e^{i\vartheta})}{\sigma(e^{i\vartheta})}. \quad (9)$$

For methods in Example 1.2, the equation $\Phi(e^{i\vartheta}, \mu) = 0$ is quadratic in μ and can be solved to obtain two root locus curves

$$[0, 2\pi) \ni \vartheta \mapsto \mu_{1,2}(\vartheta) \quad (10)$$

corresponding to the method. The root locus curve (9) or the union of the curves (10) can be plotted to yield information on $\partial\mathcal{S}$. It is often believed that the boundary of the stability region is a subset of the root locus curve.

Proposition 2.3 *Let us consider an irreducible implicit linear k -step method, that is, a method of the form (6) with $\alpha_k \neq 0 \neq \beta_k$ and the polynomials ϱ and σ having no common*

root. Let μ^* denote the unique element of \mathcal{E} in (8) and suppose that $\mu^* \in \mathcal{S}$. Then $\mu^* \in \partial\mathcal{S}$, and this μ^* is not part of the root locus curve corresponding to the method.

Proof. Due to irreducibility, we have for some $0 \leq \ell^* \leq k-1$ that the function $\mathbb{C} \setminus \{\mu^*\} \ni \mu \mapsto C_{\ell^*}(\mu)/C_k(\mu) = (\alpha_{\ell^*} - \mu\beta_{\ell^*})/(\alpha_k - \mu\beta_k)$ is not constant, where $\mu^* = \alpha_k/\beta_k = \lim_{\zeta \rightarrow \infty} \varrho(\zeta)/\sigma(\zeta)$. From the product representation $\Phi(\zeta, \mu)/C_k(\mu) = \zeta^k + \sum_{\ell=0}^{k-1} \frac{C_\ell(\mu)}{C_k(\mu)} \zeta^\ell = \prod_{m=1}^k (\zeta - \zeta_m(\mu))$ (valid for $\mu \neq \mu^*$) and from $\lim_{\mu \rightarrow \mu^*} |C_{\ell^*}(\mu)/C_k(\mu)| = +\infty$ we see that there is a root of $\Phi(\cdot, \mu)$ that is repelled to infinity as $\mu \rightarrow \mu^*$ but $\mu \neq \mu^*$. Hence $\mu^* \in \mathcal{S}$ is an isolated point of \mathcal{S} , therefore also an isolated point of $\partial\mathcal{S}$. But the image of the unit circle $\{e^{i\vartheta} : \vartheta \in [0, 2\pi)\}$ under the non-constant rational function ϱ/σ cannot contain isolated points. \square

Observation 4. Due to the presence of the exceptional set \mathcal{E} , some results on stability regions in the literature are not accurate. For example, the notion of Property C for an algebraic function determined by $\Phi(Q(\mu), \mu) \equiv 0$ has been defined in [1]. In [3, Section V.4] it is found that all one-step methods have Property C. And indeed, applying Proposition 2.7 [1] to the implicit Euler method for example, now we have that $\varrho(\zeta) = \zeta - 1$ and $\sigma(\zeta) = \zeta$ have no common root, and ϱ/σ is univalent on the set $\{z \in \overline{\mathbb{C}} : |z - 1| > 1\}$, so $Q(\mu) = 1/(1 - \mu)$ has Property C. By Corollary 2.6 and (2.21) of [1], $\partial\mathcal{S} = \Gamma := \{\mu \in \overline{\mathbb{C}} : \exists \zeta \text{ with } |\zeta| = 1 \text{ and } \Phi(\zeta, \mu) = 0\}$. Here $\Phi(\zeta, 1) = \varrho(\zeta) - \sigma(\zeta) = -1$, so $1 \notin \Gamma = \partial\mathcal{S}$. On the other hand, we have seen in (7) that $1 \in \partial\mathcal{S}$ due to definition (4).

3 Conclusion

As the above observations show, it seems reasonable from the viewpoint of numerical methods to refine the definition of the stability region as follows, affecting only the class of implicit methods.

Definition 3.1 *The stability region of a linear multistep or multiderivative multistep method with $k \geq 1$ step(s) and with stability polynomial (3) is defined as*

$$\begin{aligned} \mathcal{S} := \{ & \mu \in \mathbb{C} : \text{the degree of } \Phi(\cdot, \mu) \text{ is exactly } k, \\ & \text{all roots } \zeta_m(\mu) \text{ of } \zeta \mapsto \Phi(\zeta, \mu) \text{ satisfy } |\zeta_m(\mu)| \leq 1, \\ & \text{and multiple roots satisfy } |\zeta_m(\mu)| < 1\}. \end{aligned}$$

References

- [1] R. Jeltsch, O. Nevanlinna, Stability and Accuracy of Time Discretizations for Initial Value Problems, *Numer. Math.*, 40, 245–296 (1982)
- [2] E. Hairer, S. Nørsett, G. Wanner, Solving Ordinary Differential Equations I. Nonstiff Problems, Springer, Berlin (2009)
- [3] E. Hairer, G. Wanner, Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems, Springer, Berlin (2002)